Calculation of Global Warming Potentials

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The objectives of this project are to (1) calculate the global warming potential (GWP) of various halons that are either currently used or may be used in the semiconductor industry, and to (2) compare and contrast the GWP for these various halons in order to evaluate their relative merits with respect to their potential effect on the global environment. In order to accomplish these objectives, there was a need to calculate two quantities reliably: (1) the rovibrational transition energies, and (2) the integrated infrared (IR) band intensities.

Earth's average global temperature has been rising over the last decade, and several analyses have pointed out the global consequences of even a 2–3°Centigrade (°C) increase. Much has been said about the amount of carbon dioxide vented into the atmosphere by human activities, but the release into the atmosphere of other trace compounds such as hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), chlorofluorocarbons (CFCs), perfluorocarbons, or other halons is likely to be more important. Some of these compounds are more than 100,000 times more effective as greenhouse gases than carbon dioxide, and because of their long atmospheric lifetimes, the effects of their presence will be felt for decades. In this study, investigation of the GWP of molecules employed in the semiconductor industry, either in the manufacturing process or in the cleaning process, is undertaken. Figure 1 shows that these compounds have the potential to close the "atmospheric window" in Earth's atmosphere, leading to significant global warming.

State-of-the art methods now can calculate rovibrational transition frequencies to within a few wave numbers, more than adequate for this study, but less information is available regarding the calculation of accurate IR band intensities. Thus, the first study was devoted to the investigation of the levels of theory necessary to calculate reliable IR band intensities. This study was accomplished by first searching the literature to determine a set of benchmark CFCs and HCFCs for which reliable experimental data exist for the IR intensities of their bands that appear in the "atmospheric window." Several levels of theory have been tested. Results indicate that modest levels of theory are adequate for calculating reliable GWPs, especially considering the fact that what is most important is the relative GWPs between various molecules. Agreement between experiment and theory for the benchmark molecules was excellent.

All these compounds possess vibrational frequencies in the "window" region that have large IR intensities because of the very polar nature of the bonds involving the halogen atom (leading to large intensities) and the [force constants/atomic masses] ratio, which causes several stretching and bending frequencies to appear between 700 and 1500 per centimeter (cm^{-1}). Estimates based on the IR intensities present in the window region indicate that these compounds are among those that are 100,000 times more effective greenhouse gases than carbon dioxide.

All of these compounds, however, are not equal when it comes to GWPs. Their relative GWPs depend upon two factors: (1) the total amount of IR absorption that occurs in the window region, and (2) the relative atmospheric (tropospheric) lifetimes. Other considerations can be used in deciding which compound to use in an industrial process, such as the fact that hydroxy radical (OH) will abstract a

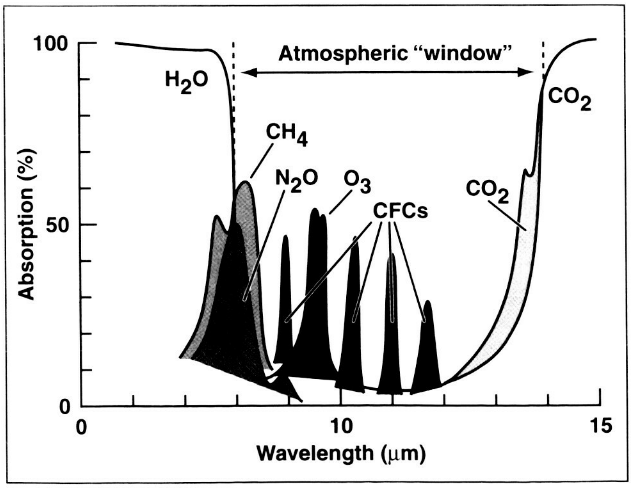

Fig. 1. Atmospheric window in the Earth's atmosphere and the absorption of IR radiation by CFCs in the window region.

hydrogen (H) atom much more readily than a halogen atom (because the second O-H bond in water is very strong relative to C-H bond energy). Consequently, HFCs and HCFCs have significantly lower tropospheric lifetimes (and GWPs) relative to similar CFCs or perfluorocarbons.

Although it will be possible to determine relative GWPs for different source gases relatively easily, all these compounds have significant GWPs (because of their large IR intensities in the window region). Hence, it is probably best for industries to adopt abatement procedures when using these types of compounds.

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Environmental Research Aircraft and Sensor Technology—New Technologies for Earth Science

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The Environmental Research Aircraft and Sensor Technology (ERAST) project is an Aerospace Technology Enterprise (NASA Headquarters Code R) program designed to provide focus for critical technology development and flight demonstration that reduces the technical and economic risk of using remotely piloted aircraft (RPA) as a means to collect scientific data in a timely and cost-effective manner. A government industry alliance (ERAST) is flying RPA in science missions with 400-pound (lb) (182 kilogram (kg)) payloads to altitudes of 55,000 feet (ft) (16.7 kilometers (km)).

Ames has the leadership role in developing sensors and science missions for ERAST. In FY99, ERAST passed a major milestone by supporting the Uninhabited Aerial Vehicle/Atmospheric Radiation Measurement (UAV/ARM) Tropical Cirrus Mission from Barking Sands, HI. Ames provided the coordination to match science needs and ERAST flight opportunities to meet this milestone. ERAST sensor support also developed one of the key instruments flown by an Ames investigator. Seven science flights were conducted during the four-week series. The total flight time above 16.7 km was 16.5 hours. Flights to 16.7 km were the highest the UAV/ARM payload has ever flown.

The ERAST Science and Sensor Element also promoted new RPA payloads and missions for atmospheric science, remote sensing, and others, including:

- Disaster management with Global Disaster Information Network (GDIN)
- Over-the-horizon (OTH) and real-time technologies for missions and vehicles
- Support of the development of the Earth Sciences Enterprise NASA Research Announcement for science and applications
- Promotion of the partnership between California Resources Agency—ARC and ERAST to systematically map California in a high-resolution sharable digital database
- Promotion of the Commercial Remote Sensing Program partnership with ERAST

The ERAST Science and Sensor Element also promoted educational and commercial outreach to support existing and planned RPA science activities at various conferences and exhibitions. One highlight included producing the Hawaii State Fair CD, which provided an overview of the ERAST, the Pathfinder, the Remote Sensing imagery from Hawaii, including flight maps, a mini-tutorial on remote sensing, and an explanation of how the imagery was acquired and manipulated. Examples of many images were provided along with simple procedures to access some 1400 images archived in Hawaii. Collaborators in this research include Susan Schoenung (Longitude 122° W), and Don Sullivan and Vince Ambrosia (Johnson Controls World Services).

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